Endrin

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 344 days

Global applicability domain: Outside

Local applicability domain index: 1.37e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

Image not found

Adamantane
Measured: 8090000
Predicted: 968

Image not found

Octahydro-exo-4,7-methano-1H-indene
Measured: 8090000
Predicted: 636

Image not found

Squalane
Measured: 5460
Predicted: 49.4

Image not found

Indeno(1,2,3-cd)pyrene
Measured: 630000
Predicted: 325

Image not found

Dibenzo[a,i]pyrene
Measured: 490000
Predicted: 311